ALCF

Argonne Leadership Computing Facility

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Overview

Pete Beckman, Director
Argonne Leadership Computing Facility

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A U.S. Department of Energy laboratory
managed by UChicago Argonne, LLC

Over 20 years of Advanced Systems for DOE and Others

- **ACRF** period [1983-1992]
  - DOE's founding ACRF
  - Explored many parallel architectures, developed programming models and tools, trained >1000 people

- **HPCRC** period [1992-1999]
  - Production-oriented parallel computing for Grand Challenges in addition to Computer Science.
  - Fielded 1st IBM SP in DOE

- **TeraGrid** [2001-present]
  - Overall Project Lead
  - Defining, deploying and operating the integrated national cyberinfrastructure for NSF
  - 9 sites, 22 systems, 200TF

- **LCRC** [2003-present]
  - Lab-wide production supercomputer service
  - All research divisions, 56 projects, 380 users

- **BlueGene Evaluation** [2005-present]
  - Founded BlueGene Consortium with IBM
    - *67 institutions, >260 members*
    - *Applications Workshop Series*
    - *Systems Software Collaborations*

ALCF Timeline

2004

– Formed of the Blue Gene Consortium with IBM
– DOE-SC selected the ORNL, ANL and PNNL teams for Leadership Computing Facility award

2005

– Installed 5 teraflops Blue Gene/L for evaluation

2006

– Began production support of 6 INCITE projects, with BGW
– Joined IBM and LLNL to design and develop next Blue Genes
– "Lehman" Peer Review of ALCF campaign plans

2007

– Increased to 9 INCITE projects; continued development projects
– Install 100 teraflops Blue Gene/P system

2008

– Begin support of 20 INCITE projects on Blue Gene/P
– Add 500T teraflops Blue Gene/P system

Mission and Vision for the ALCF

Our Mission

> Provide the computational science community with a world leading computing capability dedicated to breakthrough science and engineering.

Our Vision

> A world class center for computation driven scientific discovery that has:

- outstandingly talented people,
- the best collaborations with computer science and applied mathematics,
- the most capable and interesting computers and,
- a true spirit of adventure.
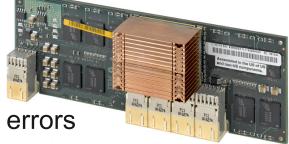
See http://www.alcf.anl.gov/ for additional information

Blue Gene DNA

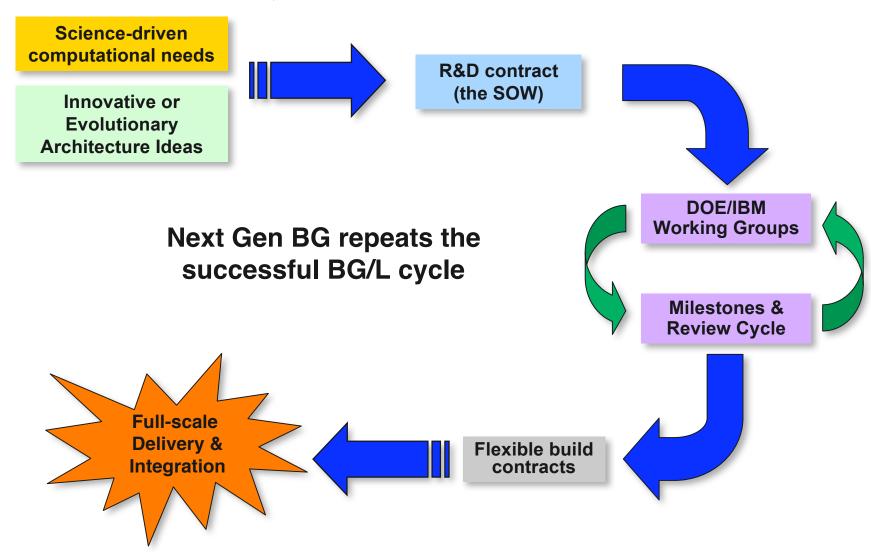- Low power design ⟹ massive parallelism
  - The leader in Green Computing
- System on a Chip (SoC)
  - Improves Price / Performance
  - Reduces system complexity & power
- Custom designed ASIC
  - Reducing overall part count, reducing errors
  - Permits tweaking CPU design to reduce soft errors
- Dense packaging
- Fast communication network(s)
- Sophisticated RAS (reliability, availability, and serviceability)
- Dynamic software provisioning and configuration

DOE / IBM Partnership for Petascale Architectures
DOE NNSA/LLNL, DOE SC/ANL and IBM/Rochester/Watson

Science-driven computational needs

Innovative or Evolutionary Architecture Ideas

R&D contract (the SOW)

DOE/IBM Working Groups

Milestones & Review Cycle

Next Gen BG repeats the successful BG/L cycle

Full-scale Delivery & Integration

Flexible build contracts

Using TAU on IBM BGP
The Open Source community is here to help…

- Choose measurement configuration

  % ls /soft/apps/tau/tau_latest/bgp/lib/Makefile.*

  > *Makefile.tau-mpi-pdt*
  > *Makefile.tau-mpi-pdt-trace*
  > *Makefile.tau-callpath-mpi-pdt*
  > *Makefile.tau-callpath-mpi-compensate-pdt*
  > *Makefile.tau-depthlimit-mpi-pdt*
  > *Makefile.tau-mpi-compensate-pdt*
  > *Makefile.tau-multiplecounters-mpi-papi-pdt*
  > *Makefile.tau-multiplecounters-mpi-papi-pdt-trace*
  > *Makefile.tau-multiplecounters-papi-pdt*
  > *Makefile.tau-multiplecounters-pthread-papi-pdt*
  > *Makefile.tau-pdt*
  > *Makefile.tau-phase-multiplecounters-mpi-compensate-papi-pdt*
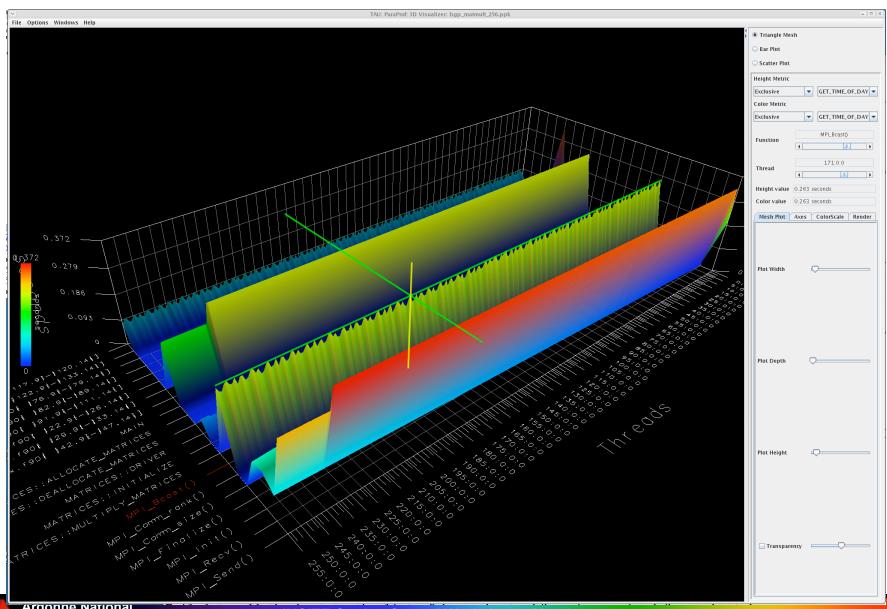 > *Makefile.tau-phase-multiplecounters-mpi-papi-pdt*
  > *Makefile.tau-pthread-pdt …*

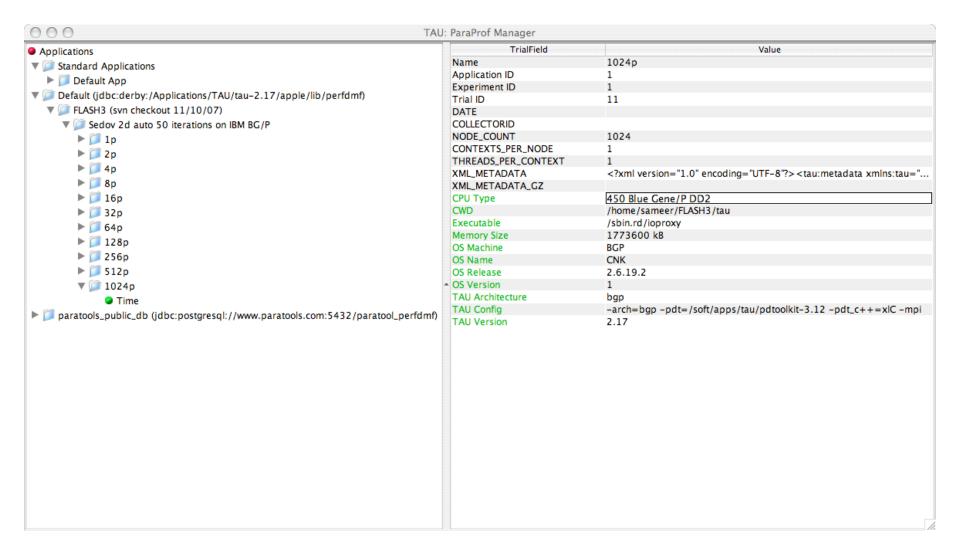 % setenv TAU_MAKEFILE /soft/apps/tau/tau-2.17/bgp/lib/Makefile.tau-mpi-pdt

  % set path=(/soft/apps/tau/tau-2.17/ppc64/bin $path)   # Front-end binaries

- Replace mpixlf90_r with tau_f90.sh and compile your application

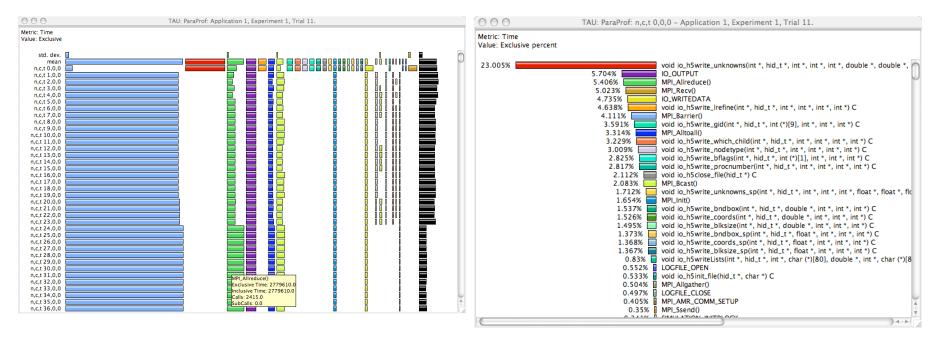 – Use tau_cxx.sh and tau_cc.sh for C++ and C compilers respectively

TAU's ParaProf 3D Profile Browser: Matmult

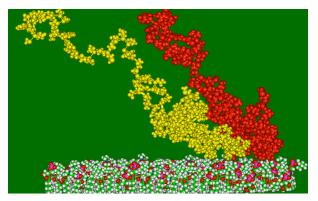# Profiling FLASH3 on IBM BG/P

Sedov 2D Auto

- Initial test run did not include a load balanced problem
- Small problem: too little work for 1024 processor
- Proof of concept to validate porting of tools

Modeling of Protofibril Structures Provides Insight into Molecular Basis of Parkinson's Disease
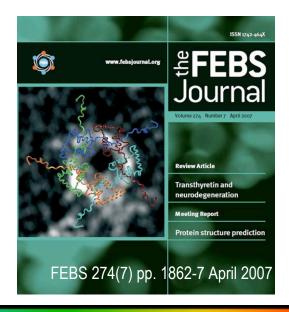## Igor Tsigelny, PI, U. California - San Diego

- Parkinson's Disease is the 2nd most common adult neurological disease

- Increased aggregation of *alpha-synuclein* protein is thought to lead to harmful pore-like structures in human membranes

- UCSD - SDSC team used molecular modeling and molecular dynamics simulations in combination with biochemical and ultrastructural analysis to show that *alpha-synuclein* can lead to the formation of pore-like structures on membranes

- Used NAMD and MAPAS on Blue Gene/L at ALCF and SDSC

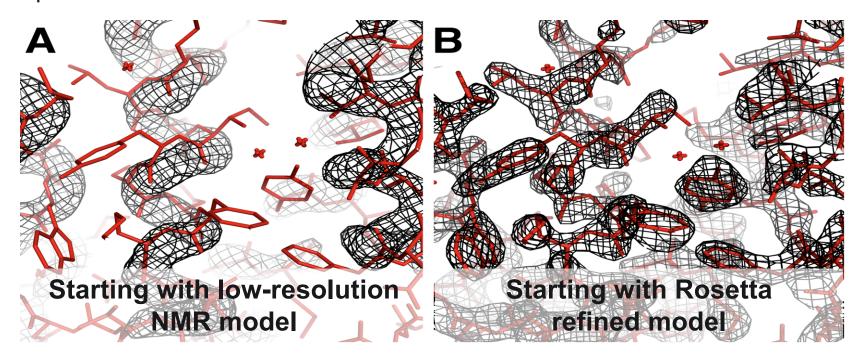*alpha-synuclein forming a dimer (above) and a completed pentamer (below) attached to a membrane*

FEBS 274(7) pp. 1862-7 April 2007

High-Resolution Protein Structure Prediction
David Baker, Srivatsan Raman, Univ. of Washington

- Proteins are the workhorse molecules of all biological systems
- ROSETTA uses a two-phase Monte Carlo algorithm to sample the extremely large space of possible structures to find the most favorable one
- Below: Electron density (black) was generated from phases determined from two starting models. The crystal structure (red) agrees very well with the phases determined from the Rosetta model.

A Starting with low-resolution NMR model

B Starting with Rosetta refined model

ALCF - ISSF, TCS

Argonne Theory and Computing Sciences Building

A 200,000 sq ft creative space to do science, Coming Summer 2009